

Last Updated 3/26/04

A Taxonomy of Hydrogen Research and Development in the U.S. Government

Prepared by the Hydrogen R&D Interagency Task Force

March 26, 2004

About the Hydrogen R&D Interagency Task Force

The Hydrogen Research and Development (R&D) Interagency Task Force was established shortly after the President's announcement of the Hydrogen Fuel Initiative in early 2003. It is co-chaired by the White House Office of Science and Technology Policy (OSTP) and the Department of Energy (DOE). The task force serves as the mechanism for collaboration among the nine Federal agencies that fund hydrogen-related research and development. The task force has developed an extensive hydrogen research taxonomy, provided guidance for agency research directions, identified key areas for interagency collaboration, and established subgroups to develop and implement a 10-year interagency coordination plan. The subgroups coordinate focused efforts in three areas:

- Fundamental Research (led by DOE's Office of Science),
- Hydrogen Production, Distribution, and Storage Technologies (led by DOE's Office of Energy Efficiency and Renewable Energy [EERE]), and
- Hydrogen Conversion Technologies (led by the Department of Commerce's National Institute of Standards and Technology).

The interagency coordination plan, to be released in 2004, will improve coordination of agency efforts, accelerate progress toward the goals of the President's initiative, and foster collaboration between the Federal government and the private sector, state agencies, and other stakeholders.

Participating agencies on the Hydrogen R&D Task Force include DOE (including Offices of EERE, Fossil Energy, Nuclear Energy, and Science), Department of Transportation, Department of Defense, Department of Agriculture, Department of Commerce, Environmental Protection Agency, National Aeronautics and Space Administration, National Science Foundation, State Department, and from the Executive Office of the President, OSTP, Office of Management and Budget, and Council on Environmental Quality. Agency research efforts address key technology barriers such as lowering the cost of hydrogen production, creating effective hydrogen storage, and developing affordable hydrogen fuel cells. The Federal agencies address these barriers by funding basic research in materials, electrochemistry, and advanced hydrogen production methods; development of components and manufacturing technologies; demonstration of systems and end-use applications; and development of safety codes and interface standards. The task force works closely with the DOE-led [International Partnership for the Hydrogen Economy \(IPHE\)](#), a collaboration among 16 nations to advance the transition to a global hydrogen economy.

About the Taxonomy

In fall 2003, the Hydrogen R&D Interagency Task Force developed a Taxonomy of Hydrogen Research and Development in the U.S. Government based on input from participating Federal agencies. In order to encourage collaboration among researchers in the public sector, private sector, academia, and the international scientific community, this taxonomy provides a structured summary of past, present, and possible future activities of the Federal government. The taxonomy is intended to provide a framework for discussion of hydrogen-related research and development. Details of funding, timing, or status have not been included. Also, in the preparation of this taxonomy, the Task Force made no attempt to evaluate the relative merit of various research approaches. Some noteworthy ideas or activities may not be adequately represented in this version. Finally, while there are many possible ways to organize such a taxonomy, the structure, format, and categories of this document reflect the specific interests and objectives of the interagency Task Force.

Table of Contents

About the Hydrogen R&D Interagency Task Force	i
About the Taxonomy.....	ii
Table of Contents.....	iii
I. Hydrogen Production	1
A. Biological Processes	1
1. Biomass Processes.....	1
2. Fermentative Production	2
3. Photobiological Production	2
4. Energy-Coupled Systems and Bioenergetics	3
5. Feedstock Production	3
6. Demonstrations.....	3
B. Fossil-Based Production	4
1. Large-Scale Gasification	4
2. CO ₂ Separation, Capture, and Sequestration.....	4
3. Distributed Production from Natural Gas or Liquid Fuels.....	5
4. On-Board Reformers	5
5. Synthesized Liquid Fuels	6
6. Demonstrations.....	6
C. Electrolytic Processes	7
1. Renewable Energy Technologies	7
2. Small-Scale Systems	7
3. Large-Scale Systems	7
4. Demonstrations.....	7
D. Advanced Thermochemical Processes	9
1. High-Temperature Water-Splitting Processes.....	9
2. Ultra-High-Temperature Water-Splitting Processes	9
3. Satellite-Based Solar Power System	9
E. Alternative Sources.....	10
1. Photocatalytic Water Splitting.....	10
2. Photoelectrochemical Water Splitting.....	10
3. Biomimetic Systems.....	10
4. Methane Splitting by Solar Energy	10
F. Hydrogen Purification	11
1. Advanced Purification Systems.....	11
2. Materials.....	11
3. Demonstrations.....	11

II. Hydrogen Transport, Distribution, and Delivery	12
A. Gaseous Hydrogen Delivery	12
1. New Pipelines.....	12
2. Existing Natural Gas Pipelines.....	12
3. Fueling Stations.....	12
4. Metering and Physical Properties.....	12
5. Procedures	13
B. Liquid Hydrogen Delivery	14
1. Liquefaction.....	14
2. Pipelines	14
3. Metering and Physical Properties.....	14
4. Demonstrations.....	14
C. Bulk Hydrogen Storage.....	15
1. Underground Storage	15
2. Gaseous Storage	15
3. Cryogenic Storage	15
III. Hydrogen Storage	16
A. High-Pressure Gas-Phase Storage	16
1. Outer/Inner Tank	16
2. Balance-of-Plant Components.....	16
3. Novel Systems	16
4. System Analysis	16
5. Demonstrations.....	17
B. Carbon Materials.....	18
1. Carbon Nanotube/Nanoparticle Design and Modeling	18
2. Manufacturing Processes.....	18
3. Novel Carbon-Related Materials.....	18
C. Metal Hydrides	20
1. Storage Materials.....	20
2. Complex Structures	20
3. Characterization of Physical Mechanisms	20
4. Containment Materials	21
5. System Analysis	21
D. Alternative Chemical Storage	22
1. Liquid Carrier Materials.....	22
2. Liquid Carrier Processes	22
3. Novel Chemical Storage Materials.....	23
4. Characterization of Physical Mechanisms	23
E. Cryogenic Storage.....	24
1. Outer/Inner Tank	24
2. Balance-of-Plant Components.....	24
3. System Analysis	24
4. Propellant Applications	25
5. Demonstrations.....	25

IV. Hydrogen Conversion	26
A. Proton Exchange Membrane Fuel Cells	26
1. Chemical Sensors	26
2. Physical System Sensors	26
3. Air and Thermal Management	27
4. Intermediate-Temperature Membranes and Stacks	27
5. System Analysis	28
B. Direct Methanol Fuel Cells	29
1. Materials and Component Design	29
2. System Analysis	29
3. Applications	29
C. High-Temperature Fuel Cells	30
1. Stack	30
2. Other Components	31
3. System Analysis	31
D. Application-Specific Technologies	32
1. Auxiliary / Portable Power Units	32
2. Stationary Applications and Distributed Power Generation	32
E. Fuel Cell Demonstrations	34
1. Light-Duty Vehicles	34
2. Medium/Heavy-Duty Vehicles	34
3. Watercraft	35
4. Aircraft	35
5. Stationary Fuel Cells	35
F. Fuel Cell Electrochemistry	36
1. Analysis	36
2. Materials and Nanotechnology	36
G. Hydrogen Combustion	38
1. Internal Combustion Engines	38
2. Turbines	38
3. Hydrogen Burning	39
V. Integrated Systems and Life Cycle Analysis	40
A. Integrated Systems Modeling	40
1. Production	40
2. Distribution and Delivery	40
3. Storage	40
4. Conversion	40
5. Well-to-Wheels Vehicular Energy and Emissions	41
6. Other Environmental and Economic Analysis	41
B. Hydrogen Infrastructure Vulnerability Analysis	42
1. Pipeline System	42
2. Ground Transport System	42
3. National Distribution System	42
C. Distributed Power Generation Systems Analysis	43
1. Vehicles	43

2. Stationary Applications	43
D. Integrated System Demonstrations.....	44
1. Power Parks	44
2. Hydrogen Production / Fueling / Vehicles	44
VI. Safety, Codes and Standards	45
A. Safety Design.....	45
1. Design Analysis for Standards Development.....	45
2. Safety-Related Sensors.....	45
3. Hydrogen Infrastructure Safety	45
4. Hydrogen Conversion Applications Safety	46
B. Safety Codes	47
1. Infrastructure Codes	47
2. Building Codes	47
C. Industry Standards.....	48
1. Applications and Components.....	48
2. Performance Standards.....	48
D. Regulatory and Enforcement Mechanisms	50
1. Vehicles	50
2. Hydrogen Transport	50
3. Weights and Measures.....	50
VII. Education	51
A. Workforce Training	51
1. End Users and Authorities.....	51
2. Other Stakeholders and Educators	51
B. Public Awareness	52
1. Consumer Information	52
2. Outreach Activities.....	52
VIII. Crosscutting Research.....	53
A. Novel Materials.....	53
1. Multifunctional materials and structures	53
2. Catalytic Materials	53
3. Hydrogen Storage Materials.....	53
4. Membrane Materials.....	53
B. Physical, Chemical, and Biological Processes in Enabling Hydrogen Research.....	55
1. Catalysis	55
2. Separations	55
3. Physical and Chemical Interactions of Materials with Hydrogen.....	55
4. Analytical and Characterization Tools	55
5. Biological and Biomimetic Hydrogen Production	55
6. Photocatalytic and Photoelectrochemical Hydrogen Production	55
C. Manufacturing Research	56
1. Large-scale Hydrogen Production and Delivery Systems.....	56
2. Component and System Fabrication.....	56

I. Hydrogen Production

A. Biological Processes

1. Biomass Processes

- a) Water-gas CO shift (WGS)
 - Goals: Production rate, Durability, efficiency of conversion, low CO in reformat
 - i. Study biological systems of WGS in order to determine alternative shift pathways.
 - Goals: Identify the relevant genetic components; Enable manipulation of gene expression.
 - ii. Single-step shift
 - Goal: Integrate WGS with membrane separation technology.
- b) Catalysts
 - Goals: Efficiency, Impurity tolerance, lower cost
 - i. WGS shift catalysts
 - ii. Reformer catalysts
 - iii. Catalysts for fluid-bed reforming of biomass pyrolysis liquid
- c) High-temperature membranes
 - Description: Requires no added catalyst.
- d) Bioreactors
 - Goals: Increase hydrogen yield to levels commercially viable.
 - i. Develop new fermentative micro-organisms.
- e) Oxygen Separation Technologies for Gasification and Reforming
 - Goals: Efficiency, Impurity tolerance
 - i. Air separation technologies
 - ii. Integrated oxygen membrane/reactor systems
- f) Pyrolysis
 - Goal: Reduce cost and improve hydrogen yield
 - i. Feedstock preparation and handling systems
 - ii. Heat integration improvements
 - iii. Vapor conditioning
 - iv. Co-product opportunities
 - v. Integrated reforming and shift processes
 - a. Demonstrate proprietary microscale reactor.
- g) Gasification
 - Goal: Reduce cost
 - i. High-pressure gasification systems (10-30 atm)
 - ii. Heat integration improvements
 - iii. Feedstock preparation and handling systems
 - iv. Integrated reforming and shift processes
- h) Gasifier product gas clean-up
 - Goals: Cost, Efficiency, Durability
 - Description: for feed into reforming operations.
 - i. Hot-gas clean-up
 - ii. Tar-cracking
- i) Catalytic steam reforming
 - Goals: Improve reforming efficiency and lower cost through improved catalysts and better integration of available heat.
 - i. Fluid-bed reforming catalysts
 - ii. Gasifier product gas reforming and conditioning catalysts
 - iii. Pyrolysis oil vapor and fractions conditioning catalysts
 - iv. Heat integration
 - v. Improved reactor configuration

j) Gas separation technologies

Description: Develop and characterize new porous materials to remove sulfur-containing compounds and carbon monoxide from the hydrogen stream.

- i. Microporous oxides
- ii. Metal-organic frameworks
- iii. Carbon sorbents

k) Thermodynamic analysis

Description: Develop a predictive model for thermodynamic properties for biomass reforming, including pressure, volume, temperature, heat capacity, viscosity, and thermal conductivity, of hydrogen + hydrocarbon (methane, ethane...) + CO₂ + alkanol (methanol, ethanol...) + water mixtures.

l) Carbon sequestration

m) Materials

Description: acidic or basic processes

n) Membrane testing

Description: Establish test methods and standard membranes to ensure reliable comparisons of gas separation technologies.

o) Aqueous-phase carbohydrate reforming

Description: This process can generate hydrogen at temperatures near 500 K via the aqueous-phase, catalytic reforming of biomass-derived oxygenated compounds such as ethylene glycol, glycerol, sugars and sugar-alcohols, which are nonflammable, non-toxic, transportable liquids. This process generates hydrogen without the need to volatilize water (and thus is more efficient than conventional steam reforming), and the water-gas shift reaction is favorable for low CO concentrations, making it possible to use a single chemical reactor.

2. Fermentative Production

Description: Includes both mesophilic and thermophilic organisms, in mixed culture anaerobic processes.

a) Nutrients

- i. Phosphogypsum

b) Reactor

Description: Develop continuous flow reactors with complex wastes.

c) Enzymatic catalysis

Description: Study hydrogenase and related enzymes wrt catalytic mechanism and sensitivity to inhibitors.

d) Genetic and metabolic pathways

- i. hydrogenotrophic (e.g., methanogens)
- ii. hydrogenogenic (e.g., sulfate-reducing bacteria)

e) Electron transfer and redox pathways

f) Novel substrates and cofactors

Description: Identify and characterize.

- i. Cellulose-rich substrates

- ii. Influence of environmental conditions such as pH, T, substrate concentration, and mixing.

- iii. Effect of germination and sporulation life cycle of clostridia.

g) Micro-organisms

Description: Identify and characterize higher-yield organisms.

- i. Develop a nucleic-acid based probe.

3. Photobiological Production

a) Molecular genetics and metabolics

Goals: Oxygen tolerance, Light-conversion efficiency, Photosynthetic electron transport efficiency

- i. Use screening methods to identify candidate photosynthetic bacteria.
- ii. Measure the specific CO shift kinetics of various photosynthetic bacteria.
 - a. Rubrivivax (Rx.) gelatinosus CBS.
 - b. cloned Chlamydomonas reinhardtii hydrogenases
- iii. Mutant hydrogenase genes
 - a. Determine which enzymes are related to O₂-tolerant mutants.
 - b. Use random or site-directed mutagenesis based on information obtained from structural analyses.

- iv. Characterize and regulate genetic and metabolic pathways.
- v. Redox potential measurement
 - Goal: Support high-throughput screening technologies.
 - Description: Develop redox potential measurement methods and provide fundamental data on enzymatic oxidation-reduction potential.
- b) Chlorophyl and other photoactive pigments
 - Goals: Optimize biophysical parameters for improved irradiance response and solar energy conversion.
- c) Enzymes
 - Description: Study enzymes with respect to sensitivity to oxygen and other inhibitors.
 - i. Hydrogenase
 - ii. Nitrogenase
 - iii. Other
- d) Electron transfer and redox pathways
 - Description: Characterization study
- e) System design
- f) Reactor design
- g) Hydrogen collection and oxygen separation technologies
- h) Gas separation technologies
- i) Analysis
 - i. Economic
 - ii. Technical

4. Energy-Coupled Systems and Bioenergetics

- a) Syntrophic associations
- b) New biological organisms and microbial communities
- c) Bioenergetics of single and mixed systems

5. Feedstock Production

- a) Forest biomass
 - Description: Short rotation wood crops, small-diameter trees
 - i. Management systems
 - ii. Economics in rural economies
 - iii. Harvest technologies
 - iv. Genetic development
 - v. Characterization
- b) Agricultural biomass
 - i. Dairy, pig farm waste
 - ii. Aquaculture farm waste
 - ii. Cheese processing waste

6. Demonstrations

- a) Fueling station
 - Description: Incorporate promising technologies into an integrated H₂ production, building power, and fueling system, at distributed locations (see V.D.2 for a complete description).
 - Goal: Evaluate efficiency, durability, and gain real-world experience.
 - i. Landfill gas feedstock cleanup
 - ii. Anaerobic digester gas feedstock
- b) Biomass gasification
- c) Biomass fermentation
- d) Algal production

B. Fossil-Based Production

1. Large-Scale Gasification

- a) Design
 - i. Multiple feedstocks
 - ii. Multiple products
 - iii. Advanced concepts
- b) Oxygen Separation Technologies for Reforming
 - Goals: Efficiency, Impurity tolerance
 - i. Air separation
 - ii. Integrated oxygen membrane/reactor systems
 - iii. Catalysts
 - iv. Materials
 - v. Ceramic-metal seals
- c) Gas Separation and Clean-up Technologies
 - Goals: Cost, Efficiency, Durability
 - Description: for feed into reforming operations
 - i. Hot-gas clean-up
 - ii. Tar-cracking
 - iii. Measurement devices
 - iv. Medium-temperature sorbents
 - v. Integrated processes
 - vi. Gas polishing
 - vii. Membrane test methods and standards
- d) Water-Gas Shift Technologies
 - i. Alternative CO shift pathways
 - ii. Catalysts
 - Goals: Efficiency, Impurity tolerance
 - a. Transient femtosecond infrared spectroscopy
 - Description: Identify transient chemical species on different catalytic surfaces to improve reaction efficiency.
 - b. Combinatorial screening using FTIR imaging
 - Description: Rapid noble-metal/metal-oxide preparation methods for high number, parallel monitoring of catalysts in small volumes.
 - iii. High-temperature membranes
 - Description: Requires no added catalyst.
 - iv. Single-step shift
 - Description: WGS integrated with hydrogen separation
- e) Materials
 - i. Acidic or basic processes
 - ii. High-temperature processing
 - iii. Low-temperature processing
- f) Hydrogen purification
 - i. Membranes
 - Goals: Temperature insensitivity, high-volume fabrication systems
 - ii. Advanced concepts

2. CO₂ Separation, Capture, and Sequestration

- a) Membranes
- b) Physical sorbents
- c) Chemical sorbents
- d) Electrochemical pumps
- e) Advanced separations
- f) Storage optimization

3. Distributed Production from Natural Gas or Liquid Fuels

Description: Small-scale, low-volume

Goals - Cost, Efficiency, Selectivity, Durability

- a) Fuel-flexible reformers
- b) Water-gas shift technology
 - Goal: Robustness over a wide range of operating conditions
 - i. Multi-step processes
 - ii. Single step shift with integral hydrogen separation
 - iii. Demonstrate proprietary reactor for one-step H₂ production and separation.
- c) Hydrogen separation technology
 - Goal: Purity sufficient for PEM fuel cells; Optimize trade-off between reformat purity and energy consumption in integrated hydrogen production/fueling system (e.g., different degrees of purity for PEM fueling vs. supply for a high-temperature fuel cell).
- d) Thermal integration of system components
- e) Alternative designs
 - Goal: Operational flexibility; Low assembly, installation, and maintenance costs
 - i. Remote facility monitoring
- f) Cost-benefit comparison of liquid fuels to natural gas
 - i. ethanol
 - ii. methanol
 - iii. sorbitol
 - iv. naphtha
- g) Operations and Maintenance
 - Goal: Reduce labor costs and spare parts requirements
 - i. Remote facility monitoring
- h) Water purity
 - Goal: Develop water purification systems that are inexpensive, effective, and durable.
- i) Carbon sequestration
 - Goal: Develop cost-effective, small-scale carbon sequestration technologies.
- j) Control strategies
 - Goal: Maximize efficiency, reduce emissions, minimize cost.
- k) Thermodynamic analysis
 - Description: Develop a predictive model for thermodynamic properties for hydrogen production, including pressure, volume, temperature, heat capacity, viscosity, and thermal conductivity, of hydrogen + hydrocarbon (methane, ethane...) + CO₂ + alkanol (methanol, ethanol....) + water mixtures.

4. On-Board Reformers

Description: 10-50-kW, fuel-flexible, including reformer, shift reactors, sulfur removal beds, CO cleanup systems, sensors, and controls.

Description: Develop a highly reliable and low-cost fuel-processing system for stationary PEMFC applications. (2002)

Goal: Reduce cost, Minimize start-up time, Reduced maintenance

- a) Reactor design
 - i. Parallel reactor warm-up
 - ii. Materials
- b) Catalysts
 - Goal: Reduce cost; Improve activity, curability under automotive operating conditions
 - i. Reforming catalysts
 - ii. Desulfurization catalysts
 - iii. Preferential catalysts
 - iv. Non-precious metal catalysts
- c) Preferential oxidation systems
 - Goal: Reduce CO from the fuel processor stream under steady state and transient operation
- d) Components
 - i. Compact steam generators

- ii. Anode tail-gas burners
- iii. Fuel pre-heaters
- iv. Compact heat exchangers
- e) Microchannels, plate reactors
- f) Alternative fuel processing techniques
- g) Waste heat minimization
- h) Testing
 - i. Steady-state operation
 - ii. Transient operation
- i) Hydrogen purification
 - Goal: Reduce CO to less than 10 ppm (< 100 ppm during transients) and remove other impurities and dilutants.
- j) Design
 - Goal: Use lower-cost materials.

5. Synthesized Liquid Fuels

- a) Computational chemistry to identify optimal, hydroge-rich formulations
- b) Distributed production technologies

6. Demonstrations

- a) FutureGen clean coal power plant
 - Description: The DOE FutureGen initiative involves construction of a 275-MW coal-power plant that will produce both electricity and hydrogen and will achieve near-zero emissions of carbon dioxide and noxious air pollutants by using carbon sequestration technologies. The plant will use the Integrated Gasification Combined Cycle process, in which the coal's carbon is converted to a "synthesis gas" made up primarily of hydrogen and carbon monoxide. The syngas is then reacted with steam to produce additional hydrogen and a concentrated stream of CO₂, at least 90% of which is captured for sequestration. The captured CO₂ will be separated from the hydrogen, perhaps by high-efficiency membranes currently under development. Initially, the hydrogen produced by the plant will be used as a clean fuel for electric power generation either in turbines, fuel cells or hybrid combinations of these technologies. The hydrogen could also be supplied as a feedstock for refineries. In the future, as hydrogen-powered automobiles and trucks are developed as part of the President's Hydrogen Fuels Initiative, the plant could be a source of transportation-grade hydrogen fuel. The project will require 10 - 15 years to complete and will be led by an industrial consortium representing the coal and power industries.
- b) Fueling station
 - Description: Incorporate promising technologies into an integrated H₂ production, building power, and fueling system, at distributed locations (see V.D.2 for a complete description).
 - Goal: Evaluate efficiency, durability, and gain real-world experience.
 - i. Natural gas feedstock

C. Electrolytic Processes

1. Renewable Energy Technologies

- a) Power conversion systems
 - i. Hybrid wind, PV/electrolysis power electronics
Goal: Cost, efficiency
 - ii. Integrated power control/grid interaction technology with electrolysis
- b) Photovoltaic cells
 - i. Manufacturing processes
 - ii. Light concentrator / PV cell modules
 - iii. Semiconductor PV cell materials
 - iv. Wide-bandgap PV materials (e.g., TiO₂)
 - a. Femtosecond-laser optical studies of electron-transfer dynamics
- c) Energy storage
 - i. Wind tower bulk storage
 - ii. Reversible solid oxide electrolyzer/fuel cell
 - iii. Dispatchable electricity generation
- d) Wind and hydropower
 - i. Analysis of low-cost hydrogen production systems
 - ii. Central production hybrid (electricity/hydrogen) systems
 - iii. Distributed production for near-term, carbon-free hydrogen
- e) Geothermal

2. Small-Scale Systems

Description: Distributed production

Goals: Cost, Durability, > 70% (LHV) system efficiency.

- a) Photovoltaic cells
 - Goal: Optimal utilization of Si or III/V solar cells in system design
 - i. Develop model to predict H₂ production using PVs
 - ii. Conduct small-scale tests

3. Large-Scale Systems

Description: Utility-scale production systems suitable for renewable-energy integration

- a) Component Design
 - Goals: Reduce O&M costs, improve durability, efficiency, high-pressure operation
 - i. Water feed
 - ii. Cell stack
 - iii. Compression
 - iv. Seals
- b) Steam Electrolysis
 - Goals: Efficiency, Electricity production cost, System durability
- c) Solid-Oxide Electrolyzer
 - Description: Reversible electrolyzer
- d) Catalysts
- e) Materials
 - Goals: Cost, Durability, Manufacturability, Efficiency, Stack compression
- f) Compression Technologies
 - Goal: Develop electrochemical, other methods integral to the cell stack to achieve output pressures > 500 psi using low-cost materials.

4. Demonstrations

Goal: Evaluate efficiency, durability, and gain real-world experience on system issues.

- a) Fueling station

Last Updated 3/26/04

Description: Incorporate promising electrolytic technologies into an integrated H₂ production, building power, and fueling system, at distributed locations (see V.D.2 for a complete description).

Goal: Evaluate efficiency, durability, and gain real-world experience.

- i. Integrate electrolytic hydrogen production into the system.

D. Advanced Thermochemical Processes

1. High-Temperature Water-Splitting Processes

Description: Redox cycles driven by solar energy or nuclear heat, operating at 700-1000 deg.C.

a) Materials

Goal: Low cost

b) Membranes and separations

c) Thermodynamic data and modeling

d) Catalysis

2. Ultra-High-Temperature Water-Splitting Processes

Description: Redox cycles driven by nuclear heat, operating at 1000-3000 deg.C.

a) Ultra-high temperature heat sources

b) Materials

c) Membranes and separations

d) Thermodynamic data and modeling

e) Catalysis

f) Nuclear reactor design

3. Satellite-Based Solar Power System

a) Ammonia / water cycle

Description: Develop thermodynamic data and models for energy, phase stability, and transport properties.

E. Alternative Sources

1. Photocatalytic Water Splitting

Description: Includes tandem photovoltaic-electrolytic processes.

- a) Light harvesting
- b) Composite and nanoscale chemical systems
- c) Interfacial chemistry
- d) Catalysis and photocatalysis
- e) Materials and characterization tools
 - i. Translucent, Hydrogen-Impermeable Materials
- f) Theory and modeling
- g) Stability and degradation mechanisms

2. Photoelectrochemical Water Splitting

- a) Semiconductor Materials
 - Goals: Cost, Durability, Efficiency
 - i. Use combinatorial or other screening methods to identify semiconductors that can meet the technical targets.
 - ii. Test new materials by placing them in operation for 1000 hrs.
 - iii. Identify and develop coatings to resist corrosion.
 - iv. Evaluate electrolyte options for improved semiconductor durability and efficiency.
 - v. Develop accelerated screening protocols to predict material durability.
- b) Hybrid systems
 - Goal: Reduce cost, improve efficiency and durability
 - i. Photochemical H₂ production using in-situ generated nano-particles
 - Description: Nano-particles can be matched to the solar spectrum.
- c) Reactor design
 - Goals: Optimize light-capture efficiency, hydrogen production, and gas collection.
- d) Light harvesting
- e) Bandgap engineering
- f) Charge transport
- g) Catalysis and photocatalysis
- h) Theory and modeling
- i) Stability and degradation mechanisms

3. Biomimetic Systems

Description: Artificial photosynthesis for water splitting

- a) Catalysts
 - i. Efficiently interface biomimetic redox catalysts into complex 2D, 3D structures for hydrogen/oxygen catalysis, sensing, and energy transduction.
 - ii. Exploit biodiversity for novel biocatalysts and determining mechanisms of assembly.
- b) Interface system
 - i. Couple electrode materials to light-driven catalytic water oxidation, hydrogen production components.
- c) Nanostructures
 - i. Develop biomimetic nanostructures to organize catalytic functions of water oxidation and hydrogen.

4. Methane Splitting by Solar Energy

F. Hydrogen Purification

1. Advanced Purification Systems

a) Pressure-swing adsorption

b) Absorption

Goals: Conductivity, Reliability

c) Zeolites

Description: Develop simplified, one-step purification of natural gas, and new processes for oxygen enrichment of air streams, using “molecular gate technology.”

2. Materials

Goal: Reduce cost

a) Molecular Sieves

Description: Extremely thin, hydrogen-selective membranes with precious metal alloys.

Goal: Stabilize membranes at high temperatures.

b) Gas separation membranes

i. Polyimide

ii. Nanocomposite polymers

iii. Organic nano polymers

c) Proton exchange oxides

Goals: Conductivity, Reliability

d) Membrane testing

Description: Establish test methods and standard membranes to support reliable comparisons of gas purification technologies.

d) Systems and Facilities

Goal: Cost, efficiency

3. Demonstrations

a) Fueling station

Description: Incorporate promising purification system technologies into an integrated H₂ production, building power, and fueling system, at distributed locations (see V.D.2 for a complete description).

Goal: Evaluate efficiency, durability, and gain real-world experience.

i. Advanced reformat purification to support fueling of PEMFC vehicles.

II. Hydrogen Transport, Distribution, and Delivery

A. Gaseous Hydrogen Delivery

1. New Pipelines

Goal: Lower cost

- a) Joining and welding technologies
- b) High-pressure materials

Goals: Reduce embrittlement, corrosion, leakage

- i. Standardized methods of testing for fracture, fatigue, stress corrosion cracking, and corrosion resistance.
- ii. Weldability of higher-grade steel (mechanized welding, inspection).
- iii. In-service inspection, integrity monitoring technologies, and risk assessment in high-consequence areas.
- iv. Composite reinforced line pipe development
- v. Polyamide plastic pipe for 500-1000 psi
 - a. material specifications
 - b. performance characterization including rapid crack propagation
- c) Coating/lining materials
- d) Seals
- e) Sensors and gas odorants
- f) Controls

2. Existing Natural Gas Pipelines

- a) Mixed hydrogen/natural gas transport
 - i. Conduct cost-benefit analysis.
 - ii. Identify technical and safety considerations.
 - a. Technical support and measurement methods to evaluate potential pipeline structural/materials degradation caused by hydrogen embrittlement.
 - iii. Hydrogen separation technologies
 - Goal: Low cost
- b) Pure hydrogen transport
 - i. Conduct cost-benefit analysis.
 - ii. Identify technical and safety considerations.
 - a. Potential pipeline structural/materials degradation caused by hydrogen embrittlement.
- c) Modeling and analysis
 - i. Effects and control of mixing contaminant gases (e.g., hydrocarbons up to C-5, sulfur odorants, pipeline constituent monomers) in hydrogen.

3. Fueling Stations

- a) Compression technologies
 - Goals: Cost, Efficiency
 - i. Develop improved compression head designs to increase suction pressure.
 - ii. Develop compression head designs to capture interstage heat loss.

4. Metering and Physical Properties

- a) Thermodynamic and transport properties
 - Description: Update and revise correlations for hydrogen thermodynamic and transport properties in both liquid and gaseous phases at temperatures from 15 K to 700 K, and pressures up to 100 Mpa.
 - Goal: Ensure equity in commercial sales of hydrogen.
- b) Thermodynamic models for mixtures of hydrogen with other compounds
 - i. hydrocarbons (e.g., methane, ethane)
 - ii. CO₂
 - iii. alkanols (e.g., methanol, ethanol)

- iv. water mixtures
- c) Disseminate codes
 - i. REFPROP database
 - ii. Chemistry WebBook
- d) Reference data for metering
 - Description: Based on physical measurements (speed of sound, dielectric constant) and including on-line analysis of mixtures.
- e) On-line gas analysis
 - i. Inherently-calibrated photoacoustic instrument

5. Procedures

- a) High-pressure compressor operation
- b) Purging and filling
- c) In-service inspection, evaluation
- d) Leak detection
- e) Federal/State code compliance

B. Liquid Hydrogen Delivery

1. Liquefaction

Goals: Cost, Efficiency

- a) Cost-benefit analysis
 - i. Large-scale operations
 - ii. Energy integration with other systems
 - iii. Improved refrigeration schemes
- b) Magnetic-caloric liquefaction
- c) Novel refrigeration technologies
 - i. Cryo-coolers

Goal: 10% improvement in efficiency
- d) Heat exchanger materials
- e) Additives to raise liquefaction temperature and liquid-phase separation

2. Pipelines

- a) Fluid-flow management
- b) Leak detection
- c) Sealing system
- d) Fluid conditioning
- e) Venting

3. Metering and Physical Properties

- a) Thermodynamic and transport properties

Description: Update and revise correlations for hydrogen thermodynamic and transport properties in both liquid and gaseous phases at temperatures from 15 K to 700 K, and pressures up to 100 Mpa.

Goal: Ensure equity in commercial sales of hydrogen.
- b) Disseminate codes
 - i. REFPROP database
 - ii. Chemistry WebBook

4. Demonstrations

- a) Airport/spaceport pipeline and fueling station
 - i. Test parameters: boil-off rate, fill and vent fluid dynamics, safety
 - ii. Autonomous operation in ambient conditions

C. Bulk Hydrogen Storage

1. Underground Storage

Description: Potentially needed for hydrogen delivery terminals, seasonal and surge capacity storage, and hydrogen production facilities.

Goal: Reduce diffusion of hydrogen, Reduce cost of storage field development

- a) Analysis
 - i. Develop tools to identify geologic structures with promising permeability characteristics.
- b) Testing
 - i. Acquire data on diffusion characteristics of underground tanks.
- c) Novel systems
 - i. Alternative cushion gases coupled with membrane separation of hydrogen.

2. Gaseous Storage

Description: Potentially needed for stationary fuel cell systems, vehicle fueling facilities, hydrogen delivery terminals, surge capacity storage, and hydrogen production facilities.

Goal: Reduce cost, Reduce venting losses

- a) Solid material storage for low-pressure hydrogen
- b) High-pressure tank materials
 - i. Metal ceramic composites
 - ii. Improved resins
 - iii. Fibers
- c) Hydrogen detection
 - i. Odorants
- d) Analysis
 - i. Life-cycle performance
 - ii. Life-cycle cost
 - iii. Durability of composite tanks
 - iv. Efficiency

3. Cryogenic Storage

Description: Potentially needed for stationary fuel cell systems, vehicle fueling facilities, hydrogen delivery terminals, surge capacity storage, and hydrogen production facilities.

Goal: Reduce cost, Reduce boil-off losses

- a) New concepts for storage-delivery systems
- b) Tank materials
 - i. Metal ceramic composites
 - ii. Improved resins
 - iii. Fibers
 - iv. Test procedures
- c) Analysis
 - i. Life-cycle performance
 - ii. Life-cycle cost
 - iii. Durability of composite tanks
 - iv. Efficiency
- d) Hydrogen detection
 - i. Odorants

III. Hydrogen Storage

A. High-Pressure Gas-Phase Storage

Goals (2010 EERE): Cost (\$67/kg-H₂ = \$2/kWh net), System Volumetric Density (0.081 kg-H₂/lit), System Gravimetric Density (9 wt%), Efficiency, Durability

1. Outer/Inner Tank

Description: 10,000 psi compressed storage tanks

a) Hydrogen-resistant liner materials

Goals: Low cost, Reduced hydrogen gas permeation, Weight, Volume, Performance

i. Metal ceramic composites

ii. Improved resins

iii. Fibers

b) Fabrication processes

c) Carbon fiber/epoxy over-wrap

i. Polymer aerogel composites

ii. Nano composite electro-spun fibers

Description: Lightweight

iii. Carbon fiber/epoxy over-wrap

iv. Clay nanocomposites

Description: Linerless tanks

Goal: Reduce hydrogen permeability

d) Conformable tank design

i. Integral reinforcements

Description: Improves mechanical strength

2. Balance-of-Plant Components

Goal: Reduce cost, Reduce weight, Enable complete and rapid refueling within material temperature constraints

a) "Smart Tank" Sensors

i. Develop early warning sensors to predict potential failures in smart tanks.

b) Leak detectors

Goals: Increase operating temperature, Reduce size, Reduce system complexity, Eliminate electrical system

i. MEMS-based

ii. Pd alloy resistors/diodes

iii. Nano-Pd resistors

iv. Silica carbide

v. Wireless

vi. Fiber optic sensors (Bragg cells)

3. Novel Systems

a) Solid-state / compressed tank hybrid

Description: Combine compressed gas technologies and reversible, solid-state storage materials.

4. System Analysis

Description: Compare compressed tanks to cryogenic, carbon, metal hydride, and chemical hydride systems for storage of hydrogen on vehicles.

a) Technical metric

i. Fuel costs

ii. Infrastructure costs

iii. Energy efficiency

iv. Weight density

v. Volume density

vi. Charge/discharge performance

- vii. Durability
- b) Testing and Life-cycle analysis
 - i. Operational factors
 - ii. Failure modes
 - iii. Safety

5. Demonstrations

- a) Fueling station
 - Description: Incorporate promising compression and storage technologies into an integrated H₂ production, building power, and fueling system, at distributed locations (see V.D.2 for a complete description).
 - Goal: Evaluate technology approaches, including costs, of mechanical and other methods of hydrogen compression to 10000 psi and stationary storage to support vehicle fueling.
 - i. Safety and security
 - ii. Failure modes and modeling

B. Carbon Materials

Goals (2010 EERE): System Gravimetric Density (>2.0 kWh/kg = 6 wt%), System Volumetric Density (>1.5 kWh/lit = 0.045 kg-H₂/lit), Cost ($< \$4$ /kWh = \$133/kg-H₂)

1. Carbon Nanotube/Nanoparticle Design and Modeling

Goals: Chemical stability (resistance to poisoning and oxidation), Resistance to segregation, Structural stability (resistance to sintering and decrepitation), Storage capacity

a) Thermodynamic performance

Description: Theoretical modeling and experimental verification

i. Finite particle size and shape effects on electronic states

ii. Physisorption models

iii. Chemisorption models

iv. Heat transport across grain boundaries

b) Heterogeneous compositions and structures

c) Catalysts

i. Catalyzed dissociation and interior storage phase

ii. Surface coating of highly reactive material, such as platinum, that can reversibly bind hydrogen with a small temperature excursion.

d) Shape, Surface, and Structure

i. Exploit the effects of curvature, shape, and pore size on surface chemistry and binding.

ii. Investigate the effects of surface morphology and defects on storage capacity.

iii. Compare crystalline and amorphous structures.

e) Adsorption capacity

Description: Theoretical modeling and experimental verification

i. Use computational chemistry models to predict the adsorption of hydrogen on single-walled carbon nanotubes.

ii. Explore large ranges of temperature, pressure, and surface morphology using a consistent metric.

iii. Establish reproducible (within 10%) measurements of carbon nanotube adsorption capacity under standard operating conditions.

f) Multilayer adsorption

Description: Investigate volumetric storage density using carbon structures at various temperatures and/or pressures, which could enable multilayer adsorption especially with novel carbon structures.

g) Cycling effects

i. Determine durability and cycling effects on hydrogen storage/release.

ii. Verify purity capabilities and tolerance to contaminants.

2. Manufacturing Processes

Description: Investigate the benefits to operating performance and storage capacity using novel processes.

Goals: Low cost, High volume

a) Mechanical milling

b) Thin film processes

c) Pretreatment

Description: Could involve sonication, acid wash, and/or heat, other factors.

3. Novel Carbon-Related Materials

Goals: Volumetric Density, Reversibility

a) Functional composites

Description: Combine different materials, using 3-D layering, that each have distinct and suitable catalytic and thermodynamic properties.

b) Doped carbon

c) Graphite

d) Metallic systems

e) High-surface-area nanoporous materials

i. Metal-organic frameworks

- ii. Aerogels
- iii. Intercalation compounds
- f) Hybrid carbon/non-carbon storage systems
- g) Fullerenes (buckyballs)

C. Metal Hydrides

1. Storage Materials

Goals: Storage/Release Temperature ($< 90^{\circ}\text{C}$), Weight Density ($> 6 \text{ wt}\%$), Cost, Reversibility, On-Board Regeneration

a) Light-metal hydrides

Description: Use combinatorial analysis to identify promising compounds.

i. Alanates

Description: Alanates generally regenerate at medium temperatures.

a. Sodium alanate (NaAlH_4)

b. Other alanates (e.g., LiAlH_4)

ii. Other compound hydrides

a. Magnesium hydrides (e.g., Mg_2NiH_4)

Description: Magnesium hydrides require high temperature for regeneration.

b. Transitional-metal-based compounds

b) Metal nitrides and imides

i. Lithium nitride

c) Novel materials

d) Synthetic metals

Description: Polymer-dispersed metal hydrides (“synthetic metals”) such as polyaniline and polypyrrole have achieved densities of 8 wt% (reported) by incorporating a low-density polymer. The polymer interacts with the metal hydride on a molecular level and also stores H_2 within the polymer structure.

2. Complex Structures

a) Nanostructures

i. Nanophase materials

ii. Nanocluster composites

iii. Develop methods to control particle size and grain size by thermal management.

iv. Theory and modeling

v. Surface modification with organic molecules

b) Microstructures

i. Multiphase intermetallics

c) Thin films

i. Multilayer film structures

ii. Amorphous film structures

3. Characterization of Physical Mechanisms

a) Hydrogen bonding

Description: Understand the fundamental atomic processes in absorption and desorption of hydrogen.

b) Lifetime degradation issues

c) Kinetics

Description: Determine the effect of the following factors on kinetics and cycling characteristics.

i. Processing

ii. Dopants

iii. Catalysts

iv. Decomposition products and chemical pathways

v. Particle size

vi. Defect sites (atomic scale)

d) Surfaces

Description: Investigate the effect of surface barriers and surface catalysts on hydrogen storage.

e) Mass transport issues

Description: Investigate the role of hydrogen-promoted mass transport on phase transformations.

f) Thermophysical properties

Description: Adjusting the lattice parameters and strains, grain structure, Fermi level, polarization, and charge distribution of the absorbents should allow tuning of the absorption potential and hence the thermodynamics of absorption. Combine experimental data with state-of-the-art characterization tools and establishment of standards for comparison.

- i. Structural
- ii. Thermodynamic
- iii. Physical
- iv. Chemical
- g) Non-thermal discharge mechanisms
 - i. Mechanical
 - ii. Chemical
 - iii. Electrical

4. Containment Materials

Goal: Cost, Durability, Compatibility with storage material

- a) Composite wall containers

5. System Analysis

- a) Cost estimates
 - i. Hydrogen storage materials
 - ii. Cryo-coolers for metal hydrides
- b) Data collection
 - i. Compile a consistent database of test results for the charge/discharge behavior of potential hydrogen storage compounds (over 2,000 compounds listed in the Sandia Hydride Information Center).
- c) Magnetic detection of diffusible hydrogen
 - Description: Magnetic and electronic measurements to quantify hydrogen availability, absorption, and desorption in various materials.
- d) Neutron scattering diagnostics
 - Description: Neutron radiation is the ideal penetrating probe for measurement and visualization of the 3-D chemical kinetics of hydrogen uptake in materials. The range of size resolutions (50 μm – 1 m) and time resolutions (100 ns – 10 fs) are sufficient for most structural and dynamic processes in hydrogen storage media. (NIST Center for Neutron Research)
 - Goal: Characterization of new hydrogen storage hydrides in terms of structure, recyclability, and storage capacity.

D. Alternative Chemical Storage

Description: Reversible chemical storage, regenerated off-board.

Goals (2010 EERE): System Gravimetric Density ($>2.0 \text{ kWh/kg} = 6 \text{ wt\%}$), System Volumetric Density ($>1.5 \text{ kWh/lit} = 0.045 \text{ kg-H}_2/\text{lit}$), Storage Cost ($< \$4/\text{kWh} = \$133/\text{kg-H}_2$), Fuel-Station Cost ($\$1.50/\text{kg}$)

1. Liquid Carrier Materials

Description: Identify and evaluate liquid carrier materials with respect to life-cycle cost, energy efficiency, hydrogen storage density, emissions, and environmental impact.

a) Hydrolysis hydrides

Description: Hydrolysis hydrides release hydrogen when added to water. This is not a directly reversible process.

Regeneration of the hydride from the hydroxide byproduct can be accomplished through a multi-step process using methane. The regeneration process is highly endothermic, relatively inefficient, and expensive. Handling and disposal of the potentially toxic byproduct in large quantities presents a further challenge.

i. Borohydrides (e.g., NaBH_4)

Description: Sodium borohydride releases hydrogen in a conversion to borax (NaBO_2).

ii. Light-metal hydrides (e.g., LiH , NaH , CaH_2 , MgH_2)

Description: These hydrides form hydroxides upon release of hydrogen.

b) Reversible liquid carriers

Description: These are hydrocarbons that can be regenerated. Characterize the energy efficiency of these processes.

i. Decalin

Description: Decalin releases hydrogen in a conversion to naphthalene at 210 deg.C .

ii. Hydrocarbons

Goal: Reduce catalyst requirements, Reduce temperature/pressure requirements

a. Benzene-Cyclohexane

b. Ethylbenzene

c) Natural gas-based carriers

Description: These liquids release hydrogen in an irreversible process.

i. Methanol

ii. Fischer-Tropsch liquids

d) Ammonia

Description: Ammonia (NH_3) can be cracked into hydrogen and nitrogen (which is released to the atmosphere) in an irreversible process at high temperatures (up to 900 deg.C at atmospheric pressure), with no co-reactants. The synthesis process requires a catalyst.

e) Novel materials

2. Liquid Carrier Processes

Description: Assess the cost, efficiency, environmental impact, safety, and feasibility of process alternatives for various liquid carriers.

a) Regeneration methods

Goals: Cost, Feasibility

i. Electrolysis

ii. Radiolysis

iii. Plasma/high energy

iv. Carbothermic processes

v. Other

b) Infrastructure requirements

i. Chemical synthesis and pretreatment

ii. Chemical dispensing / fueling

iii. Recovery of spent product (and separations)

iv. Regeneration of spent material

v. System components

c) Other process components

Goals: Cost, Efficiency, Environmental impact.

- i. Oil dispersants for slurry
- ii. Catalysts and catalyzed systems
- iii. System materials
 - a. Investigate pretreatment for caustic materials.
 - b. Evaluate durability of materials.
- iv. Synthesis of carriers
 - Goal: Effective, solvent-free synthesis approaches

3. Novel Chemical Storage Materials

- a) Organic crystals
 - Description: These crystalline materials, composed of metal-organic frameworks with a cubic, 3-D, extended porous structure, can adsorb up to 2 wt-% H₂ at room temperature and about 10 atm of pressure [*Science*, **300**, 1127 (2003)]. At lower temperatures, H₂ uptake as high as 4.5 wt-% has been reported.
- b) Amino acids
 - Description: Hydrogen might be stored efficiently using the effects of protein conformation.
- c) Clathrates and Porous materials
 - Description: In methane clathrates, a methane molecule is trapped in a cage-like ice structure at high pressure and low temperature. A similar approach might be feasible for hydrogen storage.

4. Characterization of Physical Mechanisms

- a) Hydrogen bonding
 - Description: Understand the fundamental atomic processes in absorption and desorption of hydrogen.
- b) Lifetime degradation issues
- c) Kinetics
 - Description: Determine the effect of the following factors on kinetics and cycling characteristics.
 - i. Processing
 - ii. Dopants
 - iii. Catalysts
 - iv. Decomposition products and chemical pathways
- d) Surfaces
 - Description: Investigate the effect of surface barriers and surface catalysts on hydrogen storage.
- e) Mass transport issues
 - Description: Investigate the role of hydrogen-promoted mass transport on phase transformations.
- f) Thermophysical properties
 - Description: Combine experimental data with state-of-the-art characterization tools and establishment of standards for comparison.
 - i. Thermodynamic
 - ii. Physical
 - iii. Chemical

E. Cryogenic Storage

1. Outer/Inner Tank

Goals: Low cost, Low evaporative losses, Reduced hydrogen gas permeation, Reduce boil-off

a) Materials

- i. Polymer aerogel composites
- ii. Nano composite electro-spun fibers
Description: Lightweight
- iii. Carbon fiber/epoxy over-wrap
- iv. Clay nanocomposites
Description: Linerless tanks
Goal: Reduce hydrogen permeability

v. Fabrication methods

vi. Performance analysis

b) Structural design

- i. Honeycomb structures
Goal: Increase life cycle limits
- ii. Integral reinforcements
Description: Improves mechanical strength
- iii. Vacuum jackets
Goal: Reduces polymer permeability

2. Balance-of-Plant Components

Goal: Reduce cost, Reduce weight, Enable complete and rapid refueling within material temperature constraints, Reduce boil-off

a) "Smart Tank" Sensors

- i. Develop early warning sensors to predict potential failures in smart tanks.

b) Cryo-cooler technologies

- i. Enable re-liquefaction of vapor boil-off.
- ii. Create a cryogenic shield to reduce boil-off.

c) Leak detectors

Goals: Increase operating temperature, Reduce size, Reduce system complexity, Eliminate electrical system

- i. MEMS-based
- ii. Pd alloy resistors/diodes
- iii. Nano-Pd resistors
- iv. Silica carbide
- v. Wireless
- vi. Fiber optic sensors (Bragg cells)

d) Liquid level monitoring

Description: Dip tubes

Goal: Improve accuracy

- i. State equations analysis

Description: Develop equations of state for liquid hydrogen, including the effects of important contaminants, to improve the accuracy of dip-tube level monitoring.

3. System Analysis

Description: Includes testing, modeling, and theoretical analysis.

a) Characterize failure modes in composite tanks.

b) Evaluate key factors

- i. Charge/discharge performance
- ii. Durability
- iii. Safety

4. Propellant Applications

- a) Densified hydrogen
- b) Gelled hydrogen
- c) Solid hydrogen
- d) Refrigeration technologies

Description: 15 K refrigeration systems to maintain stability of hydrogen propellant.

Goal: Efficiency

5. Demonstrations

- a) Propellant applications

Description: Test various temperatures, environmental variables, weather, vibration, angles, G-loads.

- i. Boil-off rate
- ii. Fill/vent/dump fluid dynamics
- iii. System performance
- iv. System safety
- v. Reliability
- vi. Durability

- b) Cryogenic storage / compressed dispensing fueling station

Description: Support a test fleet of commercial fuel cell vehicles.

Goals: Evaluate operation in cold climate; Evaluate the feasibility of an installation at a federal facility.

- i. Safety and security evaluation
- ii. Failure modes evaluation and modeling

IV. Hydrogen Conversion

A. Proton Exchange Membrane Fuel Cells

Description: Proton exchange membrane fuel cells (PEMFCs) work with a polymer electrolyte in the form of a thin, permeable sheet, and operate at relatively low temperatures (typically about 80 deg.C). To speed the reaction, a platinum catalyst is used on both sides of the membrane. Hydrogen atoms are ionized at the anode, and the positively charged protons diffuse through the porous membrane and migrate toward the cathode. The electrons pass from the anode to the cathode through an exterior circuit. At the cathode, the electrons, hydrogen protons and oxygen from the air combine to form water. The PEM electrolyte passes hydrogen protons and inhibits the migration of electrons and heavier gases. PEMFC efficiency is 40-50%. PEMFCs have been demonstrated in the 50-200 kW range. High-temperature (100-140 deg.C) PEMFC membranes, currently in development, would increase efficiency (by greater proton conductivity) and resistance to impurities.

1. Chemical Sensors

a) Carbon Monoxide

Description: Measure the CO concentration at the entrance to fuel cell stack, preferential oxidizer outlet, and reformer outlet.

Goals: Size, Cost

- i. Gallium nitride, integrated CO and temperature sensor
- ii. Low-temperature, amperometric devices
- iii. High-temperature devices based on proton-conducting oxides

b) Hydrogen, fuel processor outlet

Description: Measure over a wide range of concentrations and temperatures, in the presence of other constituents in the reformat stream.

c) Hydrogen, ambient

Description: Measure ambient concentrations, for safety purposes, in the presence of other species found in ambient air.

- i. Electrochemical sensors
- ii. Micro-machined thin-film sensors
 - a. Interfacial stability
- iii. Gallium nitride, integrated CO and temperature sensor
- iv. Sensors based on oxygen-conducting ceramics

d) Ammonia, sulfur compounds, and contaminants

Description: Measure concentration of H₂S, SO₂, organic sulfur compounds, ammonia, and contaminants in the presence of other constituent gases.

- i. Solid-state sensor arrays

e) Oxygen

Description: Measure oxygen concentration at the cathode exit.

g) Fuel processor sensors

Description: For reactor control

h) Reference methods and standards

Description: Accurate and uniform measurement of the concentrations of sulfur, ammonia, oxygen, carbon monoxide, and other process gases or contaminants in hydrogen.

- i. Analytical methods
- ii. Physical-property-based methods

Description: Use reference equations of state and selected properties such as speed of sound and the dielectric constant.

2. Physical System Sensors

a) Flow rate

Description: Measure flow rate of reformat or hydrogen into the fuel cell at 1-3 atm total pressure.

- i. Combine acoustic methods for gas composition and flow rate measurement.

b) Temperature

Description: Fast-response for in-situ applications, operation in high-humidity reformat streams, insensitivity to flow velocity.

c) Relative humidity

Description: For the anode and cathode gas streams, high-temperature, high-humidity operation.

Goal: <1% accuracy

i. Solid state, in-situ probes

3. Air and Thermal Management

a) Air Components

Goals: Low cost, High efficiency, Lubrication-free

i. Compressors and blowers

a. Turbo

b. Torroidal intersecting vane

c. Hybrid scroll

ii. Expanders

iii. Motors

iv. Motor controllers

b) Thermal Design

Goals: Low cost, High efficiency, Reduced size

i. Heat exchangers

ii. Condensers

iii. Heaters

iv. Radiators

v. Heat recovery systems

vi. Heat rejection materials

vii. Humidifiers

viii. Other system humidification techniques

4. Intermediate-Temperature Membranes and Stacks

Description: Operating temperature 120-200°C. New membranes are needed that provide sufficient proton and water conductivity, and lower gas permeability, at these temperatures. Access to this temperature regime would significantly improve CO tolerance, reduce the need for precious metal catalysts, and improve heat rejection in the stack – thus providing lower cost, higher efficiency and greater durability – compared to conventional, lower-temperature PEMFCs.

a) Catalysts

i. Adhesion to new polymer membranes

Description: Investigate new electrode structures and other approaches

ii. Catalyst structure and formulation

Goal: Reduce platinum loading while maintaining CO tolerance and oxygen reduction properties

a. Improve the fundamental understanding of local structure in a catalyst layer.

b. Nano- and micro-structured electrocatalyst materials

iii. Analyze effect of sulfur impurities on catalyst performance.

b) Bipolar plates

Goals: Low cost, Light weight, Corrosion-resistant, Impermeable

i. Materials

ii. Coatings

c) Membrane materials

Description: Standard, perfluorsulfonic acid-based membranes such as Nafion lose conductivity as they begin to dehydrate above 100 deg.C. New membranes are needed that provide the required proton conduction and selectivity at higher temperatures.

i. Polymeric materials

ii. Inorganic

iii. Hybrid

d) Other components

- i. Gas diffusion layer
 - ii. Seals
 - iii. Interconnects
- e) Manufacturing processes
 - i. Membranes
 - ii. Catalyst deposition
- f) Testing and Analysis
 - i. Single cell
 - ii. Sub-scale (5-10 kW) stack
 - iii. Investigate long-term stability and durability, efficiency, power density
 - iv. Standard methods and membranes to characterize performance of PEMFC membranes.

5. System Analysis

- a) Drive cycle modeling
 - Description: Simulated automotive drive and durability cycles
- b) Water management
 - i. Flow channel design
 - ii. Flow modeling
- c) System model
 - Description: Develop a validated system model, with periodic benchmarking, of the integrated fuel cell power system, subsystems, and components.

B. Direct Methanol Fuel Cells

Description: The most common type of direct hydrocarbon fuel cell is the Direct Methanol Fuel Cell (DMFC). In DMFCs, oxygen from the surrounding air is reduced at the cathode, as with PEMFCs, except that liquid methanol instead of hydrogen is the fuel oxidized directly at the anode. Thus a DMFC system does not require a hydrogen storage tank or reformer. On the other hand, by comparison to a PEMFC, a DMFC requires higher precious metal loading (higher cost) and offers lower power density, although the methanol fuel does provide higher energy density. DMFCs have been designed up to 5 kW. DMFCs may be suitable for smaller (< 0.5 kW) consumer electronics applications. A related type of fuel cell, the Direct Propane Fuel Cell, has a similar design and operating characteristics, while cryogenic propane has a higher energy density than methanol.

1. Materials and Component Design

- a) Oxidation catalysts
Goals: Resistance to methanol, Reduced Pt loading on membrane
- b) Membranes
Goal: Reduce methanol crossover; High volume, low cost manufacturing cost; Low precious-metal content
 - i. Low-cost manufacturing, including ink-jet printing of catalysts on membrane electrode assemblies.
- c) Integrated, direct hydrocarbon microcells
Description: All the components for making a micro, modular fuel cell (the electrocatalyst of cathode and anode, the separator or the membrane electrolyte, and the current collectors) can be integrated into a single fiber or cell structure. The hydrogen-containing fuel passes through each microcell connected in electrical series, resulting in a combined power production suitable for portable applications.

2. System Analysis

- a) Fluid handling
Description: Miniature technology for an on-board unit
 - i. Flow channel design
 - ii. Flow modeling
- b) System model
Description: Develop a validated system model, with periodic benchmarking, of the integrated fuel cell power system, subsystems, and components.
- c) Testing
 - i. Single cell
 - ii. Sub-scale (0.5-kW) fuel cell stack.

3. Applications

- a) Portable electronics
Description: Miniature power packs for cell phones and laptops.
 - i. Hybrid ultracapacitor-DMFC units
Description: Could provide 5x the energy density of battery packs.
- b) Stand-alone power units
Description: Direct Propane Fuel Cells for telecommunications applications.

C. High-Temperature Fuel Cells

Description: High-temperature fuel cells include solid-oxide types and molten-carbonate types. **Solid oxide fuel cells (SOFC)** use a ceramic electrolyte, which results in a solid-state unit, and operate at about 1000 deg. C. The conduction mechanism is the migration of oxygen ions from the cathode to the anode through a solid-state, crystal lattice. The reaction is completed by the reaction of oxygen ions at the anode with hydrogen (from the fuel gas) to form water, releasing electrons to the external circuit. In a **molten-carbonate fuel cell (MCFC)**, molten carbonate salts are the electrolyte. At 440 deg. C, the salts melt and conduct carbonate ions (CO_3) from the cathode to the anode. At the cathode, the electrons react with oxygen from air and CO_2 recycled from the anode to form CO_3 ions that replenish the electrolyte and transfer current through the fuel cell. At the anode, hydrogen reacts with the ions to produce water, CO_2 , and electrons that flow through the external circuit. SOFCs and MCFCs can extract hydrogen from a variety of fuels using either an internal or external reformer. Challenges for SOFC technology include increasing the power density and reducing cost, which requires improved seals and metallic interconnects. Significant technical challenges with MCFCs are the complexity of working with a liquid electrolyte rather than a solid, the inherent, relatively low power density, and high cost. A significant advantage of high-temperature fuel cells is fuel flexibility – since they are not very susceptible to CO poisoning, they can use gasified coal, natural gas, or, with minor modification, heavy fuels. Also, SOFCs and MCFCs work well with catalysts made of nickel, which is much less expensive than platinum. They can achieve an efficiency of 60% stand-alone, or up to 80% (net) if the waste heat is used for cogeneration. Currently, demonstration units exist up to 2 MW.

1. Stack

Goals: Cost reduction for manufacturing and materials, higher power density, lower temperature, and thermal cyclability.

a) Electrolyte

Description: Develop and characterize lower-temperature oxide-ion conductors. Lower-temperature operation would reduce the thermal durability problems of SOFCs and reduce material cost.

- i. Ceramics (e.g., high-strength YSZ)
- ii. Novel, synthetic solid-state materials (e.g., LSGM, doped ceria)
- iii. Multi-layer, integrated structures

b) Electrodes

Goals: Reduced thickness, Improved sulfur tolerance, CTE, Interface performance

- i. Anode – sulfur tolerance and carbon resistance
- ii. Cathode – LSM alternatives such as LSF, LSCF, SSC

c) Seals

Goals: High-temperature durability, Resistance to thermal cycling

- i. Glass composites
- ii. Ceramics

d) Interconnects

Goals: Lightweight, Oxidation resistant

- i. Ceramics
- ii. Metallics

e) Sensors

- i. Chemical Sensors
- ii. Physical System Sensors

f) Manufacturing processes

i. Cathode materials

Description: Develop a continuous manufacturing process using self-propagating, high-temperature synthesis.

- ii. Thin-film fabrication
- iii. Modular designs

Description: Develop a low-cost module that is scalable from 5 W – 5 kW.

g) Microminiaturized design

Description: For handheld electronic devices.

h) Type Casting and Calendering

i. Screen printing

- ii. Sintering
- iii. Extrusion
- iv. Deposition
- v. Plasma spray

2. Other Components

- a) Ancillaries
 - i. Pumps
 - ii. Valves
 - iii. Separators
 - iv. Interconnects
 - v. Compressors
- b) Thermal management
 - Goals: Efficiency, Size, Cost
 - i. Heat exchangers
 - ii. Condensers
 - iii. Heaters
 - iv. Radiators
 - v. Heat recovery system
 - vi. Heat rejection materials
 - vii. Humidifiers
 - viii. Other system humidification techniques
- c) Power management and distribution
 - Goals: Low EMC, High efficiency
 - i. High-power DC switching converters
 - ii. High-power, cryogenic DC switching converters
- d) Fuel processor
 - Description: Miniature units integrated with an on-board unit
 - Goals: Power density, Cost, Longevity, Tolerance of sulfur and carbon

3. System Analysis

- Description: Reliability, durability, and performance characterizations using modeling and testing.
- a) Components
 - b) Subsystems and large-scale systems
 - Description: Test steady-state, transient, and dynamic operation, in both series and parallel configurations.
 - c) Microstructure analysis
 - Description: Characterize void and phase microstructures (in the anode, cathode, and electrolyte layers, and interfaces between them) as a function of position in system materials, in order to understand control of performance properties and life-cycle changes.
 - i. X-ray synchrotron analysis
 - Description: Measure void and pore size, size distribution and connectivity, and reactivity.
 - ii. Microstructure models for SOFC performance prediction
 - d) Fueling station
 - Description: Incorporate advanced high-temperature fuel cells into an integrated H₂ production, building power, and fueling system, at distributed locations (see V.D.2 for a complete description).
 - Goal: Evaluate efficiency, durability, and gain real-world experience.

D. Application-Specific Technologies

1. Auxiliary / Portable Power Units

Description: 1-30kW systems operating at about 800°C

Goals: Cost, Specific power, Power density, Durability, Simplified fuel processing

a) Components

- i. Fluid handling
- ii. Microcompressors

b) Manufacturing processes

c) Portable fuel processors

- i. Diesel reforming

d) Fuel storage, distribution, and recharging

e) Cartridge-based systems

Description: Self-hydrating, modular PEMFC smart cartridges could increase reliability and reduce cost of small (2kW), distributed fuel cells.

f) SOFC distributed power modules

Description: 70% efficiency, 1kW and larger

g) SOFC auxiliary power units for heavy-duty trucks

2. Stationary Applications and Distributed Power Generation

Description: Size ranges from watts to megawatts.

Goals: Acceptable price point is \$400-\$750/kW for widespread commercialization. Durability requirement is 40,000 hours in temperature range -35 to 40 deg.C (several thousand hours of reliable operation has been demonstrated so far).

a) Combined heat and power with SOFCs

Description: Use the waste heat from high-temperature fuel cell for cogeneration or for a bottoming cycle. Evaluate the performance of stationary SOFCs as a steady load for integrated hydrogen production while providing a high-quality heat and power source.

Goal: Efficiency > 80%

- i. More efficient heat recovery systems
- ii. Improved system design

b) Combined heat and power with PEMFCs

Description: The low operating temperature of PEMFCs limits the use of waste heat generated by the fuel cell.

Goal: Efficiency > 80%

- i. More efficient heat recovery systems
- ii. Improved system design
- iii. Higher operating temperature

c) Integrated cooling systems

Description: Regenerating dessicants in a dessicant cooling cycle.

d) Power electronics and energy management

Goal: Cost, Efficiency, Load transient response time < 3 msec

- i. Universal DC bus
- ii. High-frequency power conditioner
- iii. Integrated transfer switch and inverter
- iv. Grid-independent electronics

e) Fast startup systems

Description: Many backup power applications require a faster startup than is currently available (at least 30 seconds) in today's fuel-cell systems.

- i. Hybrid systems (with energy storage)
- ii. Other approaches

f) Components

Goal: Increase durability to 40,000 hours.

- i. Sulfur-tolerant catalysts

- ii. Sulfur-tolerant membrane materials
- iii. Analysis of failure mechanisms
- iv. Benchmarking
- g) Marine power generation
 - Description: Demonstration of the viability of a 400-kW fuel-cell system.
 - i. Test voltage regulation, frequency regulation, load response testing, and overload testing.

E. Fuel Cell Demonstrations

1. Light-Duty Vehicles

- a) DOE Controlled Hydrogen Fleet and Infrastructure Demonstration Project
 - Description: see “Integrated System Demonstrations”
 - i. Collect data on performance, durability, and reliability.
 - ii. Identify maintenance, safety, and refueling requirements, including sensors and refueling connections.
 - iii. Collect vehicle operating experience, including fuel economy, range, cost, drivability, cold-start, emissions, and durability.
 - Description: Data will be used for modeling and composite results will be distributed.
- b) California Fuel Cell Partnership
 - Description: Provide technical guidance for the development of data acquisition systems.
- c) DOE National Validation Program
 - i. Validate vehicle performance, durability, and reliability by laboratory and in-use testing in multiple test facilities using consistent, robust test procedures.
 - ii. Evaluate design and operation of new test facilities.
 - iii. Provide detailed data to support well-to-wheels modeling efforts.

2. Medium/Heavy-Duty Vehicles

- a) UPS delivery trucks in Ann Arbor, MI
 - Description: Medium-duty delivery trucks powered by PEMFCs, conducted by EPA, DaimlerChrysler, and UPS.
 - i. Test parameters
 - a. Vehicle fuel economy (on dynamometer and in-use testing)
 - b. Fuel cell stack performance
 - i. Degradation
 - ii. Ambient temperature effects on start-up, performance and durability
 - c. Vehicle performance including cold climate and various on-road duty cycles.
 - ii. Test procedures
 - a. Develop improved standard test procedures.
 - i. Account for power management in hybrid vehicles (with battery or ultracapacitor)
 - ii. Fuel cell performance over time
 - b. Develop safety protocols for operation and garaging of commercial vehicles in a warehouse setting.
 - iii. Data collection and management
 - Description: Work with the manufacturer to collect all relevant data, protect proprietary information, and incorporate data with other data, as appropriate, for analysis of the technology baseline, progress, challenges, as well as for input to the well-to-wheels modeling efforts.
- b) Tactical wheeled vehicles
 - i. PEMFCs
 - ii. SOFCs
- c) Military trucks
 - i. Quantify emissions reductions and energy savings.
- d) Transit buses
 - i. Baseline data collection and evaluation of Gen-I fuel-cell buses
 - Description: Demos - California Fuel Cell Partnership (7 at 3 transit agencies), CUTE (27 fuel-cell buses in 9 European cities), ECTOS (3 fuel-cell buses in Iceland), STEP (3 fuel-cell buses in Perth, Australia), Japanese Fuel Cell Bus Program (2 buses in Tokyo), Canadian Fuel Cell Bus Program (1 bus in Winnipeg), Chinese Fuel Cell Bus Program. ThunderPower bus.
 - ii. Develop parameters and technical targets for Gen-II fuel-cell buses
 - a. NAVC Heavy-Duty Fuel-Cell working group
 - b. Direct input to FTA
 - c. International Fuel-Cell Bus working group
 - d. Commercial-sector R&D teams

- e. Evaluate prototypes
- e) Shuttle buses
Description: Develop and evaluate hybrid fuel cell systems (with energy storage) in light-duty shuttle buses.
- f) Locomotives
- g) FMCSA medium/heavy truck demonstration
- h) Auxiliary power units for heavy-duty trucks
Description: High-temperature fuel cells

3. Watercraft

- a) Submarines
 - i. Manned
 - ii. Unmanned
 - iii. Cryogenic oxygen storage and generation system
- b) Ferries
Description: DOT (MARAD, FHWA, FTA, and RSPA) is supporting the design, construction, and operation of fuel-cell ferries.
 - i. San Francisco – Treasure Island
Description: Compressed hydrogen, fuel cells, batteries
 - ii. Hawaii – Arizona War Memorial
Description: Compressed hydrogen, fuel cells, batteries
- c) Recreational watercraft
Description: Liquid hydride (sodium borohydride) storage, fuel cells, batteries. Seaworthy Systems is the principle developer, funding from DOD and MARAD.

4. Aircraft

- a) Long-duration, high-altitude aircraft

5. Stationary Fuel Cells

- a) Tactical field generators
 - i. PEMFCs
 - ii. SOFCs
- b) FAA airport power
- c) Remote locations
 - i. Lighthouses
 - ii. Mountain mines

F. Fuel Cell Electrochemistry

1. Analysis

Description: Basic research, applicable to many types of fuel cells.

a) Electrocatalysis

Description: Study the microstructure and reactivity of the electrocatalyst/electrolyte interface at the anode and cathode of membrane-electrode assemblies.

i. Non-linear optical techniques

Description: Vibrationally-resolved sum-frequency generation

ii. Spectroscopic in-situ probes

iii. Molecular study of reaction intermediates on catalytic surfaces.

iv. Transient femtosecond infrared spectroscopy

Description: Identify transient chemical species on different catalytic surfaces to help identify efficient reaction paths.

v. Atomistic modeling of reaction pathways

b) Sorption and transport models

Description: In membranes, models are needed for atomic-level processes (e.g., the coupled motions of polymer chains, water, and protons in polymer electrolytes), proton diffusion and transport in pores, and the relationship between macro-scale conductivity and the structure of pore networks. This helps understand performance factors and durability factors (e.g., critical membrane swelling and delamination).

i. Neutron reflectometry

ii. Small-angle scattering

c) Water distribution mapping

Description: Accurate quantification of membrane and flow-channel $\text{H}_2\text{O}/\text{H}_2$ transport dynamics using micro-scale, non-destructive visualization of spatial and temporal water distribution in the membrane, gas diffusion layer, and flow channel.

i. Neutron transmission imaging

ii. Neutron phase imaging

2. Materials and Nanotechnology

Description: Basic research applicable to many types of fuel cells, aimed at more efficiently functioning electrocatalyst-electrolyte percolation networks for membrane electrode assemblies.

a) Current collectors

Goal: Corrosion resistance

b) Nanostructures

Goals: Improve catalyst utilization, Reduce resistive losses

i. Di- and tri-block copolymers

ii. Mesoporous inorganic solids

iii. Layered thin films

c) Nanoscale catalytic centers

Description: Two-dimensional arrays of nanoscale catalytic centers could enhance the selectivity of membrane permeability, and conversely, the proximity to a selectively permeable barrier could enhance the net activity of integrated catalytic devices.

d) Selectively permeable gas diffusion layers

Description: Develop electronically conducting membranes (such as microporous carbons or hydrogen-permeable metals), or new gas diffusion layer / catalyst architectures, that selectively transport hydrogen and not CO to the catalyst surface.

e) Catalysts

Description: New cathode catalysts are needed to improve system efficiency and to reduce the heat rejection load (which could enable high-temperature PEMFCs, for example).

Goal: Cost, Durability

i. Noble-metal-based catalysts

Description: Develop and evaluate the long-term stability of catalysts other than Pt and Pt alloys that

- could provide improved mass activity (higher voltage at a given mass-specific current density).
- ii. Non-precious-metal catalysts
 - Description: Effective catalysts not based on precious metals would greatly reduce the cost of fuel cells.
 - Goal: Mass activity > 10% of Pt catalysts (in order to meet volume and weight targets).
 - a. Nanoparticles
 - iii. Fundamental analysis
 - a. Oxygen reduction reaction mechanisms on Pt and Pt alloys
 - b. Mechanisms in salt and alkaline environments (including gold)
 - c. Single crystals and surfaces of nanoparticles
 - d. Durability and degradation mechanisms
 - iv. Novel catalysts
 - Goals: Selectivity for the oxygen reduction reaction, Resistance to poisoning, Stability in the fuel cell environment.
 - a. Intermetallics
 - b. Mixed oxide-metal phases
 - c. Supported inorganic compounds
 - d. Organic compounds
 - i. Transition-metal macrocyclics
 - e. Computational modeling and combinatorial methods
 - Description: Use FTIR imaging to rapidly prepare a large number of noble-metal/metal-oxide, candidate electrocatalysts.
 - v. Novel support materials
 - Goal: Enhanced corrosion stability
 - a. Nb-doped TiO₂
 - b. Tungsten-bronzes
 - c. Stable carbons

G. Hydrogen Combustion

1. Internal Combustion Engines

Description: Spark ignition with carbureted, port, or direct fuel injection.

Goals: Efficiency, Emissions

a) Homogeneous-charge piston engines

b) Rotary engines

c) Hydrogen internal combustion engine transit bus

Description: Collaborative effort with the California South Coast Air Quality Management District and SunLine Transit.

d) Hydrogen / natural gas blended fuel bus

Description: Collaboration with SunLine Transit and UC Davis.

e) Hydrogen internal combustion engine shuttle bus

Description: Develop and evaluate a shuttle bus using a hybrid (with energy storage) hydrogen internal combustion engine with emission controls.

i. NO_x emission control system

ii. Engine calibration and testing

iii. Integration with hybrid-electric drive system

2. Turbines

a) Components

i. Lean-burn combustors

Goal: Low NO_x

a. Micro element fuel injection

b. Active control

c. Fuel injector cooling

d. Combustion diagnostics

ii. Seals

iii. Liquid hydrogen leak detectors

Goals: Increase operating temperature, Reduce size, system complexity, and electrical system

a. MEMS-based

b. Pd alloy resistors/diodes

c. Nano-Pd resistors

d. Silica carbide

e. Wireless

f. Fiber optic sensors (Bragg cells)

b) Thermal design

i. Regenerative heat exchanger

Description: for fuel conditioning

a. Materials

b. Coolant channel design

c. Manifold design

ii. Thermal barrier coatings

Goal: Increase operating temperature, Reduce coating loss due to steam environment

a. Silica carbide

b. Superalloys

iii. Blade cooling

a. Heat transfer models

c) Materials

d) Computational fluid dynamics

i. Modeling of flame speeds of hydrogen/hydrocarbon blended fuels

ii. Emissions modeling

iii. Global reaction scheme for hydrogen and blended fuels

e) Engine controls

- i. Silica carbide sensors
- ii. Wireless engine monitoring
- iii. Piezoelectric actuators
- f) Space-based applications
 - Description: Test under varying flight conditions, weather. Measure performance, emissions, dynamics, and safety.
- g) FutureGen power plant application
 - Description: Develop turbines that operate on 12 - 100% hydrogen gas, ready for commercial deployment by 2008. The blended hydrocarbon/hydrogen fuels could reduce NOx emissions. Hydrogen-driven turbines can offer higher power density and greater efficiency than hydrogen-fueled diesels. See I.B.6 for a complete description.
 - Goals: Increase efficiency (32% today), Lower firing temperature (reduces NOx emissions and enables the use of fuels with higher moisture content)

3. Hydrogen Burning

- a) Direct combustion
 - Description: Hydrogen can be used to fuel a conventional boiler similar to natural gas. The jetting must be modified to account for the different combustion velocity and increased control requirements for safe and efficient operation.
- b) Catalytic combustion
 - Description: Hydrogen enters a porous paladium/platinum plate, diffuses in the pores, and reacts catalytically to produce heat (e.g., for a building). This is more efficient and easier to control than direct combustion.

V. Integrated Systems and Life Cycle Analysis

A. Integrated Systems Modeling

1. Production

Goals: Cost analysis, market analysis, feasibility study

- a) Biological
- b) Fossil-based
 - i. Natural gas reforming
- c) Electrolytic
- d) Advanced thermochemical
- e) Power Parks (combined hydrogen and electricity production)
- f) On-board reformers

Description: for ground vehicles, fuel-cell aircraft

Goals: Analyze performance, mass/volume, component design, system design, transient/dynamic response, turndown ratio, reliability, durability

- i. Develop a system model.
- ii. Develop 1D/2D component models.
- iii. Develop a non-equilibrium reformer model.

2. Distribution and Delivery

Goals: Cost analysis, market analysis, feasibility and maintainability study, capacity analysis

- a) Pipelines
- b) Bulk transport
 - i. Port capacity
 - ii. Rail transport
 - iii. Other
- c) Distributed hydrogen refueling
- d) Combined building and hydrogen refueling systems

3. Storage

Goals: Analyze cost, mass/volume, reliability, performance, durability

- a) High-pressure gaseous storage
- b) Carbon materials
- c) Metal hydrides
 - Goals: (in addition to the above,) a transient/dynamic response model
- d) Chemical storage
- e) Cryogenic storage
 - Goals: (in addition to the above,) analyze boil-off rate

4. Conversion

Goals: Analyze cost, performance, mass/volume, component design, system design, transient/dynamic response, turndown ratio, reliability, durability

- a) Vehicular PEM Fuel Cells
 - i. Components
 - Description: Includes FC stack, heat exchanger, separator, compressor, pumps, motor
 - ii. Platinum group metals cost and availability
 - iii. Fuel processing vs. direct hydrogen fuel cell system
 - iv. Operations and maintenance costs
- b) Auxiliary Power Units
 - i. Heavy-duty truck APUs
- c) Turbines

5. Well-to-Wheels Vehicular Energy and Emissions

a) Development of modeling tool

Description: Involves at least two stages of development of a comprehensive modeling tool and ongoing improvement with actual data as it becomes available. DOE and EPA have an interagency agreement to develop this model, the first stage of which is underway, integrating DOE/Argonne's "GREET" fuel-cycle model and EPA's "MOVES" vehicle and inventory model. Model capable of projecting to 2050.

i. Stage 1 model development

Description: Stage 1 model funded to date will incorporate greenhouse gas emissions and energy consumption. Will include full menu of fuel pathways now in GREET (including hydrogen production from several sources and on several scales) and vehicle technologies including PEMFCs, hybrid PEMFCs, PEMFCs with onboard reforming, and hydrogen ICEs for cars and trucks.

ii. Stage 2 model development

Description: Stage 2, planned for the FY04-05 time frame but not yet funded, will add additional fuel pathways (including coal gasification and nuclear thermal cracking) and will add capability for regulated pollutants and air toxics at all points in the fuel-vehicle system. This stage would likely also incorporate fuel and vehicle technology cost data from V.A. (Systems Modeling)

iii. Incorporation of real-world data

Description: Ongoing incorporation of data from fuel cell vehicle and component test programs (at EPA/NVFEL and elsewhere) and fuel production/distribution/storage experience.

b) Modeling analyses

Description: Utilize the comprehensive modeling tool to perform analyses of projected impacts of various technology and market scenarios.

Goal: Support policy directions and R&D deployment within and beyond government.

i. Initial modeling analyses

Description: Will include comparisons of technology performance and cost vs. energy consumption and emissions for conventional technologies and future vehicle concepts.

6. Other Environmental and Economic Analysis

Description: Integrated analysis, including energy, emissions, and economic factors, covering the full range of hydrogen production, conversion, storage, and delivery.

a) Distributed Generation

b) Large Stationary Applications

B. Hydrogen Infrastructure Vulnerability Analysis

1. Pipeline System

Goals: Define vulnerabilities and evaluate risks. Develop preventative, protective, and emergency response measures. Provide input to regulatory and standards development processes.

- a) terrorist attack
- b) accidental damage
- c) system sensitivity to pipeline component failures

2. Ground Transport System

Goals: Define vulnerabilities and evaluate risks. Develop preventative, protective, and emergency response measures. Provide input to regulatory and standards development processes.

- a) terrorist attack
- b) accidental damage
- c) system sensitivity to specific failures

3. National Distribution System

Goals: Define vulnerabilities and evaluate risks. Develop preventative, protective, and emergency response measures. Provide input to regulatory and standards development processes.

- a) feedstock shortage
- b) terrorist attack
- c) system sensitivity to disruptions in particular modes or areas of distribution

C. Distributed Power Generation Systems Analysis

1. Vehicles

- a) Emergency vehicles with auxiliary electrical power
- b) Mobile power units

2. Stationary Applications

Description: Backup power, emergency power systems

- a) Grid interconnectivity

Description: Identify grid issues in collaboration with DEER and electric utilities.

- b) Energy management

Description: Develop strategies to cost-effectively manage various power loads by optimizing interior and exterior electrical interfaces.

D. Integrated System Demonstrations

1. Power Parks

Description: Demonstration of integrated hydrogen, power, and heat production.

- a) System elements
 - i. Stationary fuel cells
 - ii. Electrolysers
 - iii. Reversible fuel cells
 - iv. Hydrogen storage
 - v. Dispensers

2. Hydrogen Production / Fueling / Vehicles

Description: Integrated demonstrations of hydrogen production, fueling stations, and operation of fuel-cell vehicles and hydrogen combustion engine vehicles.

- a) Distributed production and fueling systems and vehicle operation
 - i. Fossil reformation
 - ii. Electrolysis
 - iii. Co-production
- b) Centralized/regional production, distribution, fueling, and vehicle operation
 - i. Renewable systems
 - ii. Fossil with sequestration
 - iii. Nuclear
 - iv. Transportation
 - v. Distribution
- c) Integrated production and fueling station

Description: An integrated system of hydrogen production, fueling, stationary fuel cell(s), hydrogen cleanup, and 10,000 psi hydrogen storage at EPA/NVFEL. (FY05-06 timeframe)

Goals: System efficiency, Cost (\$1.50 gasoline equiv.) including depreciation, Footprint, Reliability

- i. Results/Learnings
 - a. Development and evaluation of a unique control system to monitor and optimize all key operational parameters in all system components.
 - b. Demonstrate capability to maintain daily fueling of several hydrogen vehicles while testing components and systems.
 - c. Significant reduction in delivery cost for hydrogen (Target: \$1.50 per gasoline gallon equivalent, including depreciation of system components.)
 - d. Demonstrate effective heat recovery from high-temperature stationary fuel cell for reformer process, thermal compression, and building physical plant.
 - e. Demonstrate incorporation of high-temperature fuel cell into system to provide a constant sink for hydrogen production regardless of vehicle fueling demand and to generate electricity for the local grid.
 - f. Optimize hydrogen cleanup, using lower-energy cleanup for the high-temperature fuel cell and limiting higher-energy PSA cleanup to hydrogen for for fueling PEM fuel cells.
 - g. Demonstrate thermal compression of H₂ to 10,000 psi to avoid mechanical compressor.
 - h. Minimize overall station physical footprint.
 - i. Significant body of collected data on real-world performance of individual system components and the overall system.
 - j. Demonstration of renewable hydrogen sources into integrated fueling system (including biomass and/or electrolysis from "green" electricity)
 - k. Publication of results and lessons learned to support other similar efforts.
- ii. Analyze opportunities for renewable hydrogen sources for this location, including landfill gas and solar electrolysis.

VI. Safety, Codes and Standards

A. Safety Design

1. Design Analysis for Standards Development

a) Fire safety

i. Flammability

Description: Determine real-world, hydrogen flammability limits.

Goals: Support safety code development. Enable optimal system designs for safety and cost-effectiveness.

ii. Hydrogen fire analysis

Description: Simulate and analyze of the cause and nature of hydrogen fires in various scenarios.

Goals: Fire risk reduction, Non-luminous fire detection, Suppression

a. Storage

b. Transport

c. Refueling

b) Cryogenic design standards

Description: Materials are evaluated for safety and compatibility in cryogenic environments. Cryogenic hydrogen systems require unique standards.

i. Collect and review existing governmental material and vessel construction standards for hydrogen applications.

a. Reassess safety, codes, and standards based on recent alloy developments and higher volume applications.

b. Expand on existing data (including that of DOE and NASA)

Description: Some of this data is quite old and was developed for smaller-scale applications

ii. Work with industry to identify gaps, compared to expected applications, and to remedy the gaps.

2. Safety-Related Sensors

a) Hydrogen sensors

i. Electrochemical sensors

ii. Micro-machined thin-film sensors

iii. Sensors based on oxygen-conducting ceramics

iv. Chemical sensors

b) Carbon monoxide sensors

Goals: Small, Low cost

i. Gallium nitride, integrated CO and temperature sensor

ii. Low-temperature amperometric devices

iii. High-temperature devices based on proton-conducting oxides

c) Temperature

i. Fiber-optic sensors

d) Pressure

3. Hydrogen Infrastructure Safety

a) Hydrogen Storage Infrastructure

i. Piping

ii. Pressure storage vessel materials

iii. Electrical systems

b) Fueling stations

Goals: Develop certification parameters and safe design parameters, including durability limits

i. Fueling interface / nozzles

ii. Hydrogen storage tanks

iii. Automotive fueling stations

iv. Truck depots

v. Transit bus depots

vi. Marine port facilities

c) Hydrogen transport vehicles

Description: Trucks and rail

- i. Vehicle safety
 - Goals: Develop certification parameters and safe design parameters, including durability limits
- ii. Container/cylinder safety
 - Goals: Develop certification parameters and safe design parameters, including material quality and durability limits.
- d) Pipeline transport
 - i. Hydrogen leak detectors
 - ii. Pipeline integrity sensors and predictive analysis
 - iii. Risk assesment
- e) Stationary hydrogen storage
 - i. Residential
 - Goals: Define certification parameters and tests
 - ii. Commercial
 - Goals: Define certification parameters and tests
- f) Mobile hydrogen fuelers
- g) Failure Modes and Effects Analysis
 - i. Develop potential accident scenarios and key data needs.
 - ii. Establish the protocol necessary to identify failure modes and mitigate risk.
 - iii. Model failures in detail in order to predict effects.
 - iv. Develop a database of critical safety data as a reference to designers.
 - v. Develop a comprehensive textbook on the best safety management practices.

4. Hydrogen Conversion Applications Safety

- a) Portable device hydrogen storage
 - Goals: Risk assessment; Define operational limits and allowable quantity of storage for various devices and applications.
 - i. Personal use
 - ii. Commercial use
 - iii. Private transport
 - iv. Air transport
 - v. HAZMAT classification
- b) Hydrogen-powered vehicles
 - Description: Includes light-duty vehicles, heavy-duty trucks, buses, marine vehicles, and locomotives
 - Goals: Develop safe design parameters, including durability limits
 - i. Crashworthiness
 - ii. Fuel system
- c) Auxiliary power units
- d) On-board reforming units
- e) Failure Modes and Effects Analysis
 - i. Develop potential accident scenarios and key data needs.
 - ii. Establish the protocol necessary to identify failure modes and mitigate risk.
 - iii. Model failures in detail in order to predict effects.
 - iv. Develop a database of critical safety data as a reference to designers.
 - v. Develop a comprehensive textbook on the best safety management practices.

B. Safety Codes

1. Infrastructure Codes

Goals: Develop safety codes suitable for integration into local codes. Integrate draft codes into demonstration projects.

Description: Use information from R&D activity in hydrogen transport, distribution, delivery, and storage.

- a) Fueling infrastructure
- b) Garage, maintenance, and parking facilities

2. Building Codes

Description: Covers hydrogen storage, stationary fuel cells, and combined heat and power systems. Use information from R&D activity in hydrogen transport, distribution, delivery, and storage.

- a) Training
 - Description: Develop a coordinated training module suitable for all local jurisdictions.
- b) Distribution
 - Description: Define a mechanism to license standards and model codes for government distribution.
- c) Analysis and Testing
 - i. Provide defensible data for separation distances.
 - ii. Provide defensible data for underground storage.
- d) International harmonization

C. Industry Standards

1. Applications and Components

Description: Support the consensus standards process, national and international.

Goals: Enhance compatibility and market acceptance. Support, and maintain consistency with, federal rulemaking activity.

a) Vehicles

- i. Light-duty vehicles (Society of Automotive Engineers - SAE)
- ii. Heavy-duty trucks (SAE)
- iii. Buses (SAE)
- iv. Marine
- v. Rail
- vi. Aircraft (American Institute of Aeronautics and Astronautics - AIAA/NASA)

b) APU's

c) Infrastructure

- i. Fuel containers and cylinders
- ii. Fuel systems
- iii. Pipelines

d) Stationary fuel cells

- i. Test protocol for residential fuel cell systems [Electric Power Research Institute (EPRI)]

Description: The tests cover issues of efficiency, performance, and compatibility with the power grid in the case of interconnection. The final draft was delivered to EPRI in April 2002.

e) Commercial fuel transport

f) International

- i. Develop a U.S. government position and approval for international standards.
- ii. Develop a unified approach to standards development among key countries in Europe and the Pacific Rim.
- iii. Develop a mechanism to license ISO standards.

2. Performance Standards

a) Test methods

Description: Industry consensus test methodology for stationary fuel cell units.

(<http://fire.nist.gov/bfrlpubs/build01/art057.html>)

i. Identify key parameters that influence fuel cell performance

- a. environmental conditions
- b. electrical loads
- c. thermal loads

ii. Construct Fuel Cell Testing Laboratory

iii. Conduct experiments to determine effect of various parameters on overall performance

- a. Ambient temperature
- b. Relative humidity
- c. Electrical load magnitude
- d. Thermal load magnitude
- e. Transient loads

iv. Develop Consensus Test Procedure

- a. Prepare draft document
- b. Incorporate industry proposed changes/suggestions
- c. Submit draft document to American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE)/American Society of Mechanical Engineers (ASME)
- d. Revise in accordance with ASHRAE/ASME comments
- e. Publish final test procedure

b) Rating methodology

Goal: Fair evaluations for informed consumer choices about stationary fuel cells.

i. Collect performance data

- a. Various geographical locations

- b. Various electrical and thermal loads
- ii. Develop rating methodologies to predict annual performance using site meteorological and load data.
- iii. Predict annual performance and compare to measured performance.
 - a. Various geographical locations
 - b. Various electrical and thermal loads
- iv. Transfer rating methodology to fuel cell manufacturers.

D. Regulatory and Enforcement Mechanisms

1. Vehicles

- a) Safety
 - i. FMVSS (light-duty vehicles)
 - ii. GTRs - Global Technical Regulations (light-duty vehicles)
 - iii. FRA (rail)
 - iv. FMCSA (heavy-duty vehicles)
 - v. FAA (aircraft)
- b) Efficiency
 - i. NHTSA - Corporate Average Fuel Economy (CAFE) standards
 - ii. EPA - official fuel economy test procedures
 - iii. Develop hydrogen fuel consumption mass measurement procedures.
 - iv. Develop a means of accounting for, and correcting for, the effects of vehicle hybridization (i.e., energy storage) on fuel economy via high-speed current monitoring.
- c) Emissions

Description: The EPA has regulatory authority over criteria pollutants (oxides of nitrogen, carbon monoxide, non-methane hydrocarbons, and particulate matter) and other toxic air emissions. This would apply to FCVs using on-board fuel reformation.

 - i. Develop measurement techniques.
 - ii. Develop official test procedures.

2. Hydrogen Transport

- a) HAZMAT Regulations
- b) Pipeline Regulations
- c) Incident Investigation

Goal: Support rulemaking updates.

3. Weights and Measures

Goal: Assist the legal metrology community (primarily at the State level) to develop uniform device performance requirements, fair and equitable methods of measurement, and practical test procedures for commercial equipment metering of hydrogen at points of sale.

Description: Stakeholders include State Weights and Measures offices; industry manufacturers and trade associations (e.g., API, ASME, NCWM); device owners, users, and customers; and Federal (NIST) technical advisors.

- a) Issues
 - i. Specifications, tolerances, and other technical requirements for H₂ measuring systems
 - ii. Code development
 - iii. Method-of-sale requirements
 - iv. Inspection and test procedures, standards, and tolerances
 - a. Field inspections (State regulators)
 - b. Type evaluations (equipment)
 - v. Technical training
 - a. Training standards
 - b. Examinations and certifications
- b) Contexts

Description: Each requires separate activity for gaseous and liquid (cryogenic) product form

 - i. Hydrogen producers
 - ii. Pipelines and transport
 - iii. Storage facilities
 - iv. Fueling stations

VII. Education

A. Workforce Training

1. End Users and Authorities

a) Large-scale end users

Goal: Develop training tools and manuals for safe and effective operation. Develop and implement training and educational systems.

b) State and local

Goal: Educate on activity, authority, and current work; develop and implement training and educational systems.

i. Fire marshals

ii. State regulators

iii. City and County governments

iv. State government offices/representatives

c) Individual users and operators

Goal: Develop training tools and manuals for safe and effective operation. Develop and implement training and educational systems.

i. Demonstration drivers

ii. Vehicle facility operators

a. Garaging

b. Loading/unloading

iii. Refueling operators

2. Other Stakeholders and Educators

a) Technical community

Goal: Develop and implement training and educational systems, and outreach activities.

i. Corporate engineers and designers

ii. Industry consultants

iii. Suppliers

iv. Trade publications

b) Federal government

Goal: Need to educate on current activity, authority, accomplishments, and goals.

i. DOT

a. OPS inspection and regulation

b. Transportation Safety Institute

c. FMCSA user education for safety, inspection, and certification

d. FTA Fuel Cell Bus program

e. FAA pilot education

ii. Other federal agencies

ii. Congress

c) Future technical workforce

Goals: Develop and implement curricula for students and training systems for educators. Support internships on fuel-cell vehicle testing and evaluation.

i. K-12

ii. Community colleges – 2-year technician degrees

iii. Undergraduate – Baccalaureate degrees

iv. Graduate – Masters and PhD degrees

Description: EPA/NVFEL is discussing a cooperative agreement with Univ. of Michigan on graduate student internships.

v. Postdoctoral education

B. Public Awareness

1. Consumer Information

- a) Information clearinghouse and website
- b) Public perceptions assessment
Description: Assess perceptions with respect to hydrogen safety, fuel-cell benefits, market challenges, and consumer values.

2. Outreach Activities

- a) Public education campaign
Description: Use fact sheets, press releases, open houses, public workshops, and public displays. Consider outreach methods at the state and local level as well as for regional, national, and international audiences and venues. Topics could include safety, ease of operation, availability, emissions and efficiency information, and other consumer benefits.
 - i. Fuel cell vehicles
 - ii. Hydrogen fueling stations
- b) Partnerships with governmental and non-governmental organizations
Description: Use vehicle demonstrations, safety education, and disseminating information on fuel-cell operation and benefits.
 - i. State fire marshals

VIII. Crosscutting Research

A. Novel Materials

1. Multifunctional materials and structures

Description: Designing and achieving multi-functionalities in a system by materials engineering or by integrating materials with different properties and structures.

a) Hydrogen separation/sensing

Description: Discover materials that could provide both hydrogen gas separation and sensing.

b) Hydrogen production/conversion

Description: Design materials and structures that could produce hydrogen and generate electrical power simultaneously.

c) Hydrogen production/storage/conversion

Description: Combine the functionalities of hydrogen production, storage and conversion in a system or a single device to reduce mass and to increase efficiency by mimicking nature.

2. Catalytic Materials

Description: Develop non-platinum / non-noble-metal-based catalysts with potential applications in hydrogen production, storage, and conversion, including electrolysis, photoelectrochemical and photochemical production techniques, fuel cell electrodes and reformers. Areas of focus include more efficient, carbon-resistant reforming catalysts; more active, low-temperature-shift catalysts; better electrolysis catalysts; better photocatalysts; more efficient removal of contaminants, including sulfur and carbon monoxide; more CO-resistant anode materials for PEMFCs; better cathode materials with lower overpotentials for PEMFCs; development of hydrogen activation catalysts that depend less on noble metals; and multifunctional catalysts.

a) Catalytic mechanisms

Goals: Understand the following fundamental issues: catalytic activity from one system to the next; selectivity and trends in selectivity; deactivation mechanisms; the chemical and structural state of the active site during catalysis; metal-support interactions; size effects in catalysts; metal-metal interactions in bi- and multi-metallic catalysis; and methods for designing novel micro- and mesoporous solids.

i. Theory and modeling of catalytic properties

ii. Nano- to atomic-scale characterization methodologies

iii. High-throughput combinatorial synthesis and screening techniques

b) Nanoscale structures

Description: Controlled synthesis of nanomaterials with tailored structures can produce novel categories of catalysts with high surface area and a large, controllable concentration of catalytic active sites.

c) Fabrication techniques

Description: Including nanofabrication technology.

3. Hydrogen Storage Materials

Description: Chemical stability, storage capacity, reversibility, thermodynamics of uptake and discharge, regeneration of irreversible materials, nanoscale effects, reproducibility of synthesis and performance, understanding of structure/function relationships

a) Carbon-based materials

b) Complex metal hydrides

c) Novel Materials and processes

d) Chemical hydrogen storage

4. Membrane Materials

Description: Potential applications in hydrogen production, storage, and conversion, including electrolyzers, gas separation systems, hydrogen purification, sensors, and fuel cell electrolytes.

a) Selectively permeable membranes

Description: Could yield efficient, inexpensive solar-to-hydrogen energy conversion devices as well as efficient electrode interfaces for fuel cells.

b) High-temperature membranes

Description: An ability to conduct efficient separations at high temperatures and in corrosive environments could enable high-efficiency solar or nuclear thermochemical water splitting. High-temperature, high-conductivity membranes could enable more efficient, low-cost, and durable fuel cells.

B. Physical, Chemical, and Biological Processes in Enabling Hydrogen Research

Description: Understand fundamental materials science to support broader discoveries of new materials for hydrogen production, storage, and conversion components.

1. Catalysis

- a) Nanoscale catalysts
- b) Innovative synthetic techniques
- c) Novel characterization techniques
- d) Theory, modeling, and simulation of catalytic pathways

2. Separations

- a) Integrated nanoscale architectures
- b) Fuel cell membranes
- c) Porous separation media
- d) Theory, modeling and simulation of separation processes and materials

3. Physical and Chemical Interactions of Materials with Hydrogen

- a) Thermodynamics and kinetics of hydrogen-materials interactions
- b) Chemical and physical stability and degradation mechanisms
- c) Surfaces and interfaces

4. Analytical and Characterization Tools

- a) In-situ characterization
- b) Electrochemical processes monitoring
- c) Neutron-based techniques
- d) Dynamic, high spatial and temporal resolution techniques
- e) Sensors

5. Biological and Biomimetic Hydrogen Production

Description: Direct production of hydrogen using biological organisms or bio-inspired materials

- a) Biological enzyme catalysts
- b) Biological and bio-hybrid energy coupled systems
- c) Theory, modeling and nanostructure design

6. Photocatalytic and Photoelectrochemical Hydrogen Production

- a) Photocatalysis
- b) Light harvesting and photoconversion concepts
- c) Organic and inorganic semiconductors

C. Manufacturing Research

1. Large-scale Hydrogen Production and Delivery Systems

- a) Measurements and standards
 - i. Methods
 - ii. Tools
 - iii. Data
- b) Process optimization and control
 - Goals: Safety, Reliability, Cost
 - i. Processes and equipment
 - ii. Assembly techniques
 - iii. Manufacturing control

Description: Unit process control, including the incorporation of intelligence into control and sensing systems to optimize and/or automate production.
- c) System integration

2. Component and System Fabrication

- Description: The fundamental process and infrastructure technologies needed to transition hydrogen products, including fuel cells, into high volume production
- a) Metrology, testing, and quality standards
 - b) High-speed and high-quality fabrication and assembly methods
 - c) Modeling and simulation
 - d) Cost-effective integration of components, subsystems and systems